Table 20A-7-001. SbSI. Unit cell parameters [Å] from different sources [64Arn, 74Ito, 76Ito].

T [°C]	a	b	c	Ref.
1.3	8.52_5	10.13_7	4.09_7	76Ito
6	8.52_3	10.12_4	4.11_1	64Arn
27	8.522(3)	10.130(4)	4.088(2)	74Ito
35	8.52_7	10.13_8	4.08_9	64Arn
48	8.533(3)	10.169(4)	4.090(2)	74Ito

Table 20A-7-002. SbSI. Fractional coordinates and anisotropic temperature parameters at $T = -185$ °C, 16 °C and 100 °C [76Iwa]. B_{ij} is defined by Eq. (a) in Introduction.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
	$T = -185$ °C								
Sb	0.1204(3)	0.1230(3)	0.2860(–)	0.0011(3)	0.0015(2)	0.0055(10)	–0.0008(5)	0.0004(5)	–0.0002(5)
S	0.8435(6)	0.0481(5)	0.2363(–)	0.0027(5)	0.0020(3)	0.0113(21)	–0.0007(9)	–0.0007(9)	0.0014(11)
I	0.5083(4)	0.8287(2)	0.2189(–)	0.0022(3)	0.0015(2)	0.0071(11)	–0.0015(6)	0.0000(6)	0.0002(6)
	$T = 16$ °C								
Sb	0.1195(2)	0.1238(2)	0.2544(–)	0.0037(2)	0.0039(2)	0.0304(12)	–0.0005(2)	0.0086(19)	–0.0009(20)
S	0.8448(3)	0.0468(4)	0.2478(–)	0.0041(3)	0.0051(3)	0.0248(21)	–0.0002(3)	0.0059(56)	0.0001(35)
I	0.5088(2)	0.8284(2)	0.2463(–)	0.0053(2)	0.0033(2)	0.0185(10)	–0.0004(2)	–0.0035(25)	–0.0001(20)
	$T = 100$ °C								
Sb	0.1195(4)	0.1239(3)	0.25	0.0051(4)	0.0048(2)	0.0388(15)	–0.0006(4)		
S	0.8443(6)	0.0471(4)	0.25	0.0062(8)	0.0054(4)	0.0174(22)	0.0004(6)		
I	0.5095(4)	0.8280(3)	0.25	0.0069(5)	0.0039(2)	0.0191(11)	–0.0011(4)		

Table 20A-7-003. SbSI. Fractional coordinates and temperature parameters at 1.3 °C [76Ito]. U_{ij} [Å^2] is defined by Eq. (d) in Introduction.

	Sb	S	I
x	0.12022(8)	0.8450(2)	0.50854(7)
y	0.12335(6)	0.0472(2)	0.82839(5)
z	0.27519(34)	0.2547(13)	0.25
U_{11}	0.0146(2)	0.0104(7)	0.0196(2)
U_{22}	0.0184(2)	0.0123(7)	0.0149(2)
U_{33}	0.0254(3)	0.0139(8)	0.0161(2)
U_{12}	–0.0026(2)	0.0009(5)	–0.0029(2)
U_{13}	–0.0003(5)	0.0014(16)	–0.0008(5)
U_{23}	0.0011(5)	–0.0017(17)	–0.0009(4)

Table 20A-7-004. SbSI. Fractional coordinates and temperature parameters at 27 °C and 48 °C [74Ito]. b_{ij} is defined by Eq. (b) in Introduction.

	27 °C			48 °C		
	Sb	S	I	Sb	S	I
x	0.1198(1)	0.8453(3)	0.5085(1)	0.1197(1)	0.8447(3)	0.5086(1)
y	0.1232(1)	0.0468(2)	0.8281(1)	0.1232(1)	0.0469(2)	0.8281(1)
z	0.25	0.25	0.25	0.25	0.25	0.25
b_{11}	0.00477(7)	0.00381(20)	0.00652(7)	0.00528(7)	0.00455(23)	0.00702(8)
b_{22}	0.00407(5)	0.00320(15)	0.00324(4)	0.00452(6)	0.00307(15)	0.00358(4)
b_{33}	0.03562(39)	0.01921(96)	0.01892(23)	0.03777(43)	0.02034(103)	0.02127(26)
b_{12}	–0.00076(5)	–0.00008(1)	–0.00069(5)	–0.00086(5)	0.00020(15)	–0.00080(5)

Table 20A-7-005. SbSI. Interatomic distances at 35 °C and 5 °C [67Kik]. See Fig. 20A-7-006 for the numbers assigned to the atoms.

Interatomic distances [Å]		
phase	I	II
Sb(III)–S(IV)	2.764(21)	2.605(27) 2.835(28)
Sb(III)–S(III)	2.492(26)	2.475(17)
Sb(III)–I(I)	3.098(5)	2.987(11) 3.247(12)
Sb(III)–I(IV)	3.813(6)	3.714(10) 3.926(10)
S(III)–S(IV)	3.551(21)	3.516(19)
S(IV)–I(I)	4.084(19)	4.071(17)
S(IV)–I(II)	3.713(16)	3.691(23) 3.741(23)
S(IV)–I(IV)	3.620(19)	3.631(18)
S(IV)–I(III')	3.815(16)	3.812(23) 3.860(22)
I(I)–I(IV)	4.546(7)	4.548(6)
I(I)–I(II')	4.052(5)	4.043(4)

Table 20A-7-006. SbSI. Interatomic distances and bond angles at T = –185 °C, 16 °C and 100 °C [76Iwa]. See Fig. 20A-7-005 for the numbers assigned to the atoms.

	–185 °C	16 °C	100 °C
Sb(1)–S'(1)	2.525(30) Å	2.468(3) Å	2.477(5) Å
Sb(1)–S(1)	2.536(13)	2.681(3)	2.715(3)
Sb(1)–S(2)	2.878(11)	2.723(3)	2.715(3)
Sb(1)–I(1)	2.918(14)	3.094(2)	3.126(3)
Sb(1)–I(2)	3.308(13)	3.138(2)	3.126(3)
Sb(1)–Sb'(2)	3.796(17)	3.829(2)	3.860(3)
S(1)–I'(1)	3.696(25)	3.726(3)	3.739(4)
S(1)–Sb(1)–I(1)	95.33(55)°	88.68(8)°	88.07(11)°
S(2)–Sb(1)–I(2)	81.21(46)	87.05(8)	88.07(11)
Sb(1)–S(2)–Sb(2)	98.91(63)	99.05(10)	98.72(14)
Sb(1)–I(1)–Sb(2)	82.61(37)	82.53(5)	82.43(9)

Table 20A-7-007. SbSI. Interatomic distances and bond angles at 1.3 °C [80Ito].

Sb(1)–Sb(2)	3.828(1) Å	S(1)–Sb(1)–S'(1)	98.78(11)°
Sb(1)–S(1)	2.761(4)	S(1)–Sb(1)–S(2)	83.13(11)
Sb(1)–S(2)	2.472(2)	S(1)–Sb(1)–I(1)	85.65(8)
Sb(1)–S(3)	3.851(2)	S(2)–Sb(1)–I(1)	81.58(9)
Sb(1)–I(1)	3.186(1)	S(2)–Sb(1)–I'(1)	83.84(9)
Sb(1)–I(4)	3.858(1)	I(1)–Sb(1)–I'(1)	82.08(2)
Sb(1)–I'(4)	3.747(1)	S(2)–Sb(2)–S(1)	85.84(11)
Sb(2)–S(2)	2.634(4)	S(2)–Sb(2)–I(2)	90.71(9)
Sb(2)–I(2)	3.051(1)		
S(1)–S(2)	3.479(5)		
S(1)–I(2)	3.715(3)		
S(1)–I(3)	3.846(3)		
S(1)–I(4)	3.626(2)		
S(2)–I(1)	3.736(3)		
S(3)–I(1)	3.866(3)		

Table 20A-7-008. SbSI. Elastic constant $c_{\lambda\mu}^{\boldsymbol{D}}$ measured by Brillouin scattering [70San].

$c_{\lambda\mu}^{\boldsymbol{D}}$ [$\cdot 10^{10}$ N m^{-2}]	Paraelectric phase ≈ 22 °C	Ferroelectric phase ≈ 12 °C
c_{11}	3.09(9)	3.06(9)
c_{22}	3.27(4)	3.14(4)
c_{33}	4.95(6)	5.18(6)
c_{44}	2.21(3)	2.24(3)
c_{55}	0.92(3)	0.99(3)
c_{66}	0.60(2)	0.59(2)
c_{12}	0.96(9)	0.85(9)
c_{13}	0.93(30)	0.97(30)
c_{23}	1.58(12)	1.44(12)